

1,1,1,3,3,3-Hexafluoropropan-2-yl trifluoroacetate

42031-15-2 | DTXSID80340673

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.69

Global applicability domain: Inside

Local applicability domain index: 3.77e-01

Confidence level: 5.50e-01

Nearest Neighbors from the Training Set

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Hexafluoroacetone

Measured: 1.46

Predicted: 1.55

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1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-

Measured: 3.30

Predicted: 3.01

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Ethyl perfluoropropionate

Measured: 2.12

Predicted: 2.04

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Perflenapent

Measured: 4.40

Predicted: 4.23